Probing atomic-scale structures and at electrochemical interfaces using in-situ x-ray diffraction

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The importance of electrochemistry in the development of many key technologies, particularly in energy conversion and storage, has highlighted the need for a fundamental understanding of the atomic structure at the electrochemical interface both in the solid electrode side and into the liquid electrolyte [1]. This is because changes in the atomic structure across the electrochemical interface induced by changes in the applied electric field strongly correlate with both activity and stability. Although electrochemical reactions always involve charge transfer processes, the applied potential can also induce structural rearrangement without charge transfer [2]. Examples include processes such as metal surface relaxation and surface reconstruction but also double layer charging which leads to rearrangement on the electrolyte side of the interface. Electrochemical surface science is a field that has grown both from theoretical and experimental advances, the latter driven by the development of techniques that can probe the electrode structure under the electrolyte and during electrochemical reactions, known as in-situ or operando measurements. Surface x-ray diffraction (SXRD) utilizing synchrotron x-ray radiation has been prominent in the study of single crystal metal surfaces in the electrochemical environment and has been particularly successful in identifying structural changes on the metal side of the interface. In terms of ordering in the liquid side of the interface, measurement and modelling of the specular crystal truncation rod (CTR) scattering is one of the few methods that can probe the entire interface structure.

Recent advances have allowed to gain additional insight into the charge distribution [3-5], the structure of the electrolyte at the interface [6] and time resolved structural development [7].

Examples of how the use of surface x-ray scattering techniques can help to characterise electrochemical interfaces in-situ in order to link, structure, reactivity and stability will be presented. [2-4]

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